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2.2.4.3 Anesthetic Concentration of Haloalkanes; 2.2.4.4 Odor Sensitivity of Pyrazines; 2.2.5 Conclusions; References; 3 Experimental Design in Synthesis Planning and Structure-Property Correlations; 3.1 Experimental Design; 3.1.1 The Importance of Experimental Design in Medicinal Chemistry; 3.1.2 Strategy in Experimental Design; 3.1.3 Selected Methods for Experimental Design; 3.1.3.1 Methods for the Direct Optimization of Lead Compounds; 3.1.3.2 Methods for the Systematic Investigation of Parameter Space; 3.1.3.3 Choice of Molecular Descriptors; 3.1.4 Summary and Conclusion; References; 3.2 Applications of Statistical Experimental Design and PLS Modeling in QSAR; 3.2.1 Introduction; 3.2.2 A Strategy for QSAR Development in Drug Design; 3.2.2.1 Formulation of Classes of Similar Compounds (Step 1); 3.2.2.2 Structural Description and Definition of Design Variables (Step 2); 3.2.2.3 Selection of the Training Set of Compounds (Step 3); 3.2.2.4 Biological Testing (Step 4); 3.2.2.5 QSAR Development (Step 5); 3.2.2.6 Validation and Predictions for Non-Tested Compounds (Step); 3.2.3 Examples of Design and PLS Modeling; 3.2.3.1 Bradykinin Potentiating Pentapeptides; 3.2.3.2 Dipeptides (Inhibiting the Angiotensin Converting Enzyme); 3.2.3.3 Dipeptides (Bitter Tasting); 3.2.3.4 Mimetics; 3.2.3.5 Haloalkanes; 3.2.3.6 Dibenzofurans; 3.2.3.7 Monosubstituted Benzenes; 3.2.3.8 Corrosive Carboxylic Acids; 3.2.4 Discussion and Conclusions; Software Used; Acknowledgements; References; 3.3 Total Response Surface Optimization; 3.3.1 Background; 3.3.2 Representation of a Response Surface; 3.3.3 Structure Descriptors from Chemical Graph Theory; 3.3.4 Examples; 3.3.4.1 Neurotoxicity of Fluorophosphorous Compounds; 3.3.4.2 Bioconcentration of Chlorinated Phenyls and Biphenyls

Sommario/riassunto

The statistical analysis of experimental and theoretical data lies at the heart of modern drug design. This practice-oriented handbook is a comprehensive account of modern chemometric methods in molecular design. It presents strategies for making more rational choices in the planning of syntheses, and describes techniques for analyzing biological and chemical data. Written by the world's experts, it provides in-depth information on* molecular concepts* experimental design in the planning of syntheses* multivariate analysis of chemical and biological data* statistical validation